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An acceptance diagram analysis of the contaminant pulse removal problem with direct geometry neutron chopper spectrometers

J.R.D. Copley*

NIST Center for Neutron Research, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899-8562, USA

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Abstract

Phased choppers are used to produce pulsed beams of monochromatic neutrons at research reactors and spallation neutron sources. Depending on the design of the instrument, it is very possible that the choppers will transmit neutrons with wavelengths other than those within the desired band of wavelengths. One or more additional choppers are typically needed to remove these contaminant pulses. We describe a method of determining the wavelength- and time-dependent transmission of a system of choppers using acceptance diagrams. The method is illustrated with calculations for the Disk Chopper Spectrometer at the NIST Center for Neutron Research and the proposed Cold Neutron Chopper Spectrometer at the Spallation Neutron Source (Oak Ridge, TN).

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Keywords: Neutron scattering; Time-of-flight; Neutron choppers; Acceptance diagrams

1. Introduction

At a number of neutron scattering centers, phased choppers are used to produce pulsed beams of low energy monochromatic neutrons. A continuous source requires at least two choppers. The first ("pulsing") chopper creates bursts of polychromatic neutrons and the second ("monochromating") chopper (ideally) selects neutrons within a given band of wavelengths from those that pass through the first chopper. In practice several, if not many, discrete wavelength bands with significant intensity would be transmitted, in addition to the desired band of wavelengths. The unwanted ("contaminant") wavelengths are typically removed by locating a third chopper between the principal (pulsing and monochromating) choppers. In some situations, it may be necessary to employ more than one contaminant-removal chopper to ensure that the transmitted beam is clean. The situation is similar at a pulsed neutron

*Tel. +1-301-975-5133; fax: +1-301-921-9847.
E-mail address: john.copley@nist.gov (J.R.D. Copley).

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source, except that the pulsing chopper(s) may or may not be required depending on the extent to which the source itself fulfills that role.

In designing direct geometry chopper instruments, it is crucial to determine how many choppers are needed to remove contaminant pulses, and where to place them. To the author's knowledge, this matter was first discussed more than 40 years ago in a paper by Lowde [1], who argued that for vanishingly short chopper open times, the ratio (d'/d), where d' is the distance from the pulsing chopper to the intermediate chopper and d is the distance from the pulsing chopper to the monochromating chopper, should be an "irrational fraction". Lowde also discussed an approach to choosing (d'/d) in the more realistic situation where the open times of the principal choppers cannot be ignored. His analysis was extended by Scherm and Springer [2] in a report that addresses the applications and physical layout of a multiple chopper spectrometer located at a source of cold neutrons. This instrument eventually materialized as the IN5 time-of-flight spectrometer at the Institut Laue-Langevin in Grenoble, France [3].

The time-of-flight instruments "Mibemol" at the Laboratoire Léon Brillouin (Saclay, France) [4], and NEAT at the Hahn-Meitner Institut (Berlin, Germany) [5,6] also use multiple choppers. Lechner [5] used a numerical method, combined with practical considerations, to determine where to place contaminant-removal choppers in the NEAT spectrometer, and a somewhat similar approach was adopted in designing the Disk Chopper Spectrometer (DCS) at the NIST Center for Neutron Research [7].

In recent years there have been additional studies. Schober et al. [8] described an analytical approach to the problem and applied their method to the design of the chopper system for the upgraded IN5 spectrometer. Narehood et al. [9] studied the implications of chopper placement at a pulsed neutron source instrument, applying their methods to the Cold Neutron Chopper Spectrometer (CNCS) that is to be installed at one of the beam lines of the Spallation Neutron Source (SNS) in Oak Ridge, TN.

In this paper we describe an analytical approach using the concept of acceptance diagrams [10]. The method is introduced in Section 2 and in the following section we present the results of calculations for the DCS and CNCS instruments. Our conclusions are summarized in Section 4.

2. Acceptance diagrams

Our objective is to determine the transmission properties of a system of choppers. If the source is pulsed it itself is identified as the first chopper. Each chopper (including the source if pulsed) is treated as an idealized device whose transmission is unity for a single-valued open time and zero for a single-valued closed time. The open and closed times add up to the repetition time. The inverse of the repetition time is the pulse frequency which is an integer multiple of the chopper frequency. All pulse frequencies are integer multiples of an overall system frequency. The system repeat time is the inverse of the system frequency.

2.1. Two choppers

We first consider a very simple system that comprises two choppers with identical repetition times T and open times $2w$, phased to transmit neutrons of wavelength λ_0. Fig. 1 is a time–distance diagram that illustrates such a system. The time of flight between the two choppers for neutrons with wavelength λ_0 is $\tau_0 d$, where d is the distance between the choppers, $\tau_0 = \lambda_0 m_n/h$ is the inverse velocity of neutrons with wavelength λ_0, m_n is the mass of the neutron and h is Planck's constant ($h/m_n \approx 3.956$ Å mm/μs).

Each neutron that arrives at the first chopper is characterized by its wavelength λ or its inverse velocity $\tau = \lambda m_n/h$, and by its time at the first chopper, t_1. With no loss in generality, we define the origin of time so that the first chopper is open at all times t_1 that satisfy the pair of conditions

$$n_1 T - w \leqslant t_1 \leqslant n_1 T + w, \tag{1}$$

where n_1 is an integer. It follows that chopper 2 is open at all times t_2 that satisfy

$$\tau_0 d + n_2 T - w \leqslant t_2 \leqslant \tau_0 d + n_2 T + w, \tag{2}$$

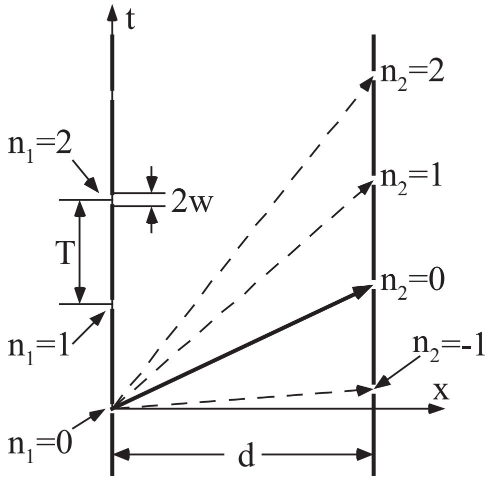

Fig. 1. A time–distance (t, x) diagram for a pair of identical choppers with period T and open time $2w$, separated by the distance d. Arrows represent possible neutron trajectories originating at one of the open times of the first chopper. Of these, the desired neutron trajectory is represented by the arrow that connects open times labeled $n_1 = 0$ and $n_2 = 0$. The slope of this line, dt/dx, is the inverse velocity of the desired neutrons, τ_0. In general the desired neutrons have $n_1 = n_2$ and the contaminants have $n_1 \neq n_2$.

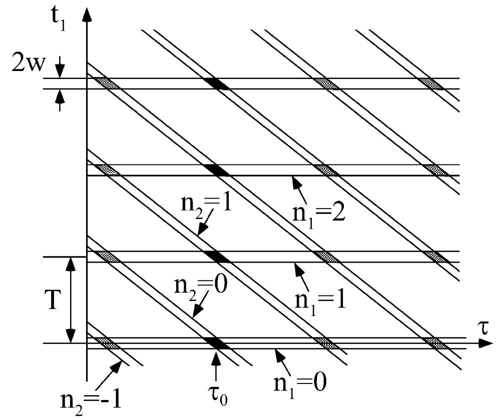

Fig. 2. A portion of the acceptance diagram for the system shown in Fig. 1. Any point on this plot represents a neutron whose inverse velocity is τ and whose time at chopper 1 was t_1. The space between each horizontal (sloping) line pair corresponds to neutrons transmitted by the first (second) chopper. Line pairs are labeled according to the transmitting chopper and open time. The light and dark solid areas represent neutrons transmitted by both choppers. The desired neutrons, with $\tau \approx \tau_0$, are represented by the dark solid areas. The gradient of the sloping lines is $dt_1/d\tau = -d$.

where n_2 is an integer. A neutron with inverse velocity τ, whose time at the first chopper is t_1, reaches the second chopper at the time $t_2 = t_1 + \tau d$. Hence, Eq. (2) may be rewritten as

$$(\tau_0 - \tau)d + n_2 T - w \leqslant t_1 \leqslant (\tau_0 - \tau)d + n_2 T + w. \quad (3)$$

The only neutrons that pass through the two choppers are those that satisfy both pairs of conditions on t_1, Eqs. (1) and (3). The situation is represented graphically as an acceptance diagram in Fig. 2. The conditions on t_1 correspond to pairs of lines and the neutrons that satisfy both pairs of conditions, i.e. those that are accepted, are represented by the shaded polygons. Each polygon corresponds to a specific choice of n_1 and n_2. The desired neutrons, with inverse velocities centered at τ_0, satisfy $n_1 = n_2$ and appear in the second column of polygons (in this example). Clearly, neutrons with inverse velocities centered at $\tau_n = \tau_0 + nT/d$, where n is a nonzero integer such that $\tau_n > 0$, will also be transmitted (if found in the incident beam). Many of these contaminant neutrons can be removed using an additional chopper.

2.2. Multiple choppers

Consider now a system of N choppers ($N \geqslant 2$). Proceeding from the source, successive choppers are numbered $k = 1, \ldots, N$. The repetition time of chopper k is T_k, its open time is $2w_k$, and the distance between choppers k and ℓ is $d_{k\ell}$; $d_{k\ell} > 0$ for $k < \ell$. The choppers are phased to transmit neutrons of wavelength λ_0, inverse velocity $\tau_0 = \lambda_0 m_n/h$. The time origin is defined as before, and chopper k is therefore open at all times t_k that satisfy the pair of conditions

$$\tau_0 d_{1k} + n_k T_k - w_k \leqslant t_k \leqslant \tau_0 d_{1k} + n_k T_k + w_k, \quad (4)$$

where n_k is an integer. Since for any given neutron $t_k = t_1 + \tau d_{1k}$, we obtain

$$(\tau_0 - \tau)d_{1k} + n_k T_k - w_k \leqslant t_1 \leqslant (\tau_0 - \tau)d_{1k} + n_k T_k + w_k \quad (k = 1, \ldots, N), \quad (5)$$

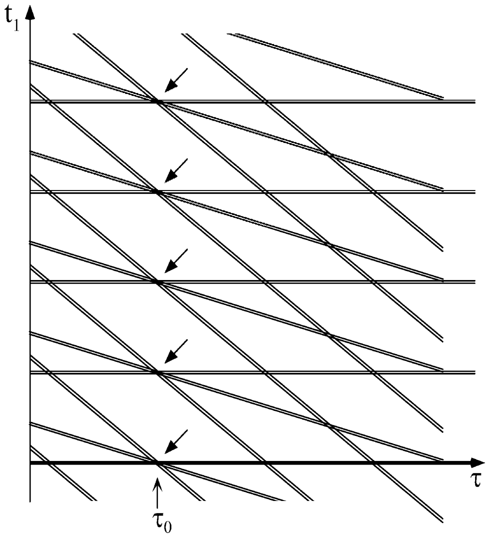

Fig. 3. A portion of the acceptance diagram for the system shown in Fig. 1, with an additional chopper placed at an intermediate position in order to remove contaminant neutrons. The transmitted (accepted) neutrons have (t_1, τ) coordinates that lie between three line pairs with different slopes. The accepted areas are indicated by the arrows.

which is a set of N pairs of conditions that t_1 and τ must satisfy in order for neutrons to be transmitted by all of the choppers. Note that Eq. (5) can equally be written as a set of N pairs of conditions to be satisfied by t_ℓ (the time at chopper ℓ) and τ:

$$\tau_0 d_{1\ell} + (\tau_0 - \tau) d_{\ell k} + n_k T_k - w_k \leqslant t_\ell \leqslant \tau_0 d_{1\ell} + (\tau_0 - \tau) d_{\ell k} + n_k T_k + w_k \quad (k = 1, \ldots, N). \tag{6}$$

Fig. 3 is an acceptance diagram similar to Fig. 2, showing the effects of adding an intermediate chopper to the two chopper system discussed in the previous subsection. Arrows pinpoint locations where three line pairs intersect, corresponding to the accepted neutrons. For the range of inverse velocities shown in Fig. 3 all other neutrons are removed.

3. Calculations and results

The acceptance diagram for a system of N choppers (subject to the restrictions noted in the first paragraph of Section 2) may be plotted in more than one way, depending on the choice of ordinate. We choose t_1 as the ordinate, in which case the acceptance diagram is constructed from multiple line pairs

$$t_1 = (\tau_0 - \tau) d_{1k} + n_k T_k \pm w_k \tag{7}$$

with slope $-d_{1k}$ and intercept $\tau_0 d_{1k} + n_k T_k \pm w_k$. Each line pair is associated with a unique pair of values of k and n_k. The (t_1, τ) coordinates of the accepted (transmitted) neutrons correspond to points located between N line pairs, one for each value of k. For a given system of choppers, we wish to determine whether or not any neutrons are accepted, other than those centered at the desired inverse velocity (or wavelength) and time(s) at the first chopper. Since what matters is the difference $|\tau - \tau_0|$, equivalently $\Delta\lambda = |\lambda - \lambda_0|$, and since wavelength is more commonly discussed than inverse velocity, we shall express the results of our calculations in terms of $\Delta\lambda$.

Given the temporal periodicity of the system, we need only consider the $p_1 = T_0/T_1$ pulses from the first chopper that occur within the system repeat time T_0. For example, if $p_1 = 1$, it suffices to consider intersections of sloping line pairs (with $k > 1$) with the single horizontal line pair $t_1 = \pm w_1$. More generally, we would consider p_1 successive pulses centered at times $t_1 = n_1 T_1$ with $n_1 = 0, \ldots, p_1 - 1$, or we could consider $p_k = T_0/T_k$ successive pulses at chopper k, centered at times $t_k = \tau_0 d_{1k} + n_k T_k$ with $n_k = 0, \ldots, p_k - 1$. In what follows, the relative intensity of a given contaminant, I, is expressed as a ratio of areas, A/A_0, where A is the acceptance area for the contaminant neutrons and A_0 is the acceptance area for the desired neutrons (with $n_k = 0$ for $k = 1, \ldots, N$).

3.1. Results for the DCS

We have studied the behavior of the DCS chopper system, omitting one member of each of the pulsing and monochromating chopper pairs and ignoring the frame overlap chopper. Thus, the DCS was conservatively modeled as a system of four choppers with $T_k = T_0 = 3000$ μs for $k = 1, \ldots, 4$ (all choppers spinning at ≈ 333 Hz). The distances d_{1k} for $k = 1, \ldots, 4$ are 0, 3.956, 6.616

and 9.004 m, respectively, and the open times $2w_k$ (identified as the time from first opening to final closing) are 175, 242, 225 and 142 μs for $k = 1, \ldots, 4$, respectively. These times were evaluated by writing $2w_k = T_k(\theta_k + \theta_G)/2\pi$, where θ_k is the full angular width of the chopper slot (12°, 20°, 18° and 8° for $k = 1, \ldots, 4$) and $\theta_G \approx 9°$ is the maximum angle subtended by the guide at the rotational axis of the chopper, determined from the width of the guide (30 mm) and the distance of its inside top surface from the rotational axis (190 mm).

Initially leaving out the intermediate choppers we find that the system transmits all neutrons within wavelength bands centered at $\lambda = \lambda_0 + n\,\delta\lambda$, where n is any integer such that $\lambda > 0$. The quantity $\delta\lambda = (T_0/d_{14})(h/m_n)$ is roughly 1.3 Å and the system is clearly useless.

A single intermediate chopper removes most of the contaminant neutrons. With chopper 2 in place, but chopper 3 "removed", we find eight contaminant regions within the range of $\Delta\lambda$ from 0 to 80 Å; the region with the smallest $\Delta\lambda$ has $\Delta\lambda \approx 11.8$–11.9 Å and $I \approx 0.33$. Conversely, with chopper 3 in place and chopper 2 "removed", there are seven contaminant regions within the same range of $\Delta\lambda$; the region with the smallest $\Delta\lambda$ has $\Delta\lambda \approx 5.3$ Å and $I \approx 0.003$. With both intermediate choppers, the only contaminant in the same range of $\Delta\lambda$ occurs at $\Delta\lambda \approx 44.8$ Å with $I \approx 0.021$ ($n_k = 0$, 15, 25 and 34 for $k = 1$, 2, 3 and 4, respectively).

3.2. Results for the CNCS

We have also performed calculations relevant to the CNCS project, to be compared with the results reported by Narehood et al. in Ref. [9]. In this case the source (which is the SNS moderator) operates at 60 Hz, and 600 Hz pulse-shaping choppers were placed 5 and 30 m from the source. An additional 60 Hz chopper was located between the 600 Hz choppers. The so-called "t_0" chopper, which blocks the beam during the release of very high-energy radiation from the source, was not included. Thus, the CNCS was modeled as a system with $N = 4$, $T_0 = T_1 = T_3 = 16666.7$ μs and $T_2 = T_4 = 0.1T_0$. Following Narehood et al. [9], we set $2w_1 = 600$ μs and $2w_3 = 1000$ μs.

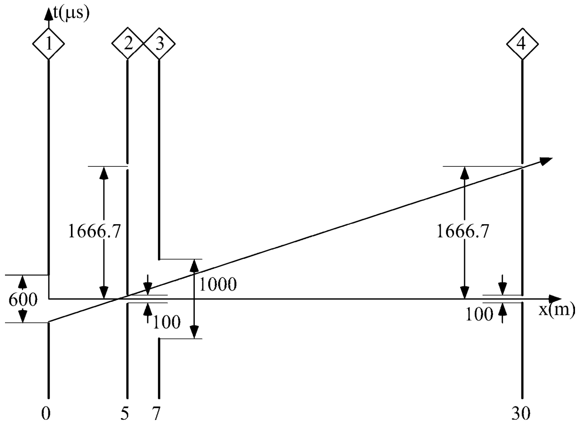

Fig. 4. A (t, x) diagram for the chopper system discussed in Ref. [9] with $d_{13} = 7$ m, showing how contaminant neutrons with $n_1 = n_2 = n_3 = 0$ and $n_4 = 1$ are produced.

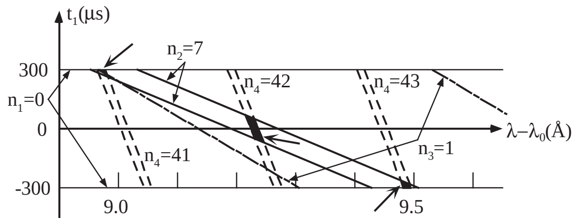

Fig. 5. A portion of the acceptance diagram for the chopper system discussed in Ref. [9] with $d_{13} = 7$ m, showing the production of contaminants with $n_1 = 0$, $n_2 = 7$, $n_3 = 1$ and $n_4 = 41$, 42 and 43. Pairs of lines, analogous to those shown in Figs. 2 and 3, are labeled appropriately. Heavy arrows point at the contaminated regions.

The open times for the 600 Hz choppers are generally small. Using $2w_2 = 2w_4 = 10$ μs the first contaminant region, i.e. the region with the smallest $\Delta\lambda$, occurs at $\Delta\lambda \approx 9.23$, 33.0 and 2.64 Å, with $I = 1.0$ in all cases, for $d_{13} = 7$, 24 and 25 m, respectively. Increasing $2w_2$ and $2w_4$ to 100 μs, the first contaminant is unchanged for $d_{13} = 25$ m, whereas with $d_{13} = 24$ m the first contaminant now has $\Delta\lambda \approx 5.5$ Å with $I \approx 0.22$ ($n_k = 0$, 4, 2 and 25 for $k = 1$, 2, 3 and 4, respectively), and with $d_{13} = 7$ m the first contaminant now appears at $\Delta\lambda \approx 0.25$ Å, again with $I \approx 0.22$ ($n_1 = n_2 = n_3 = 0$, $n_4 = 1$); the latter situation is illustrated in Fig. 4. The next three contaminants (with $d_{13} = 7$ m and

$2w_2 = 2w_4 = 100$ μs) have $\Delta\lambda$ between ≈ 9.0 and ≈ 9.5 Å with $I \approx 0.09$, 1.0 and 0.22. These contaminants, shown in the time–wavelength acceptance diagram of Fig. 5, have $n_1 = 0$, $n_2 = 7$, $n_3 = 1$ and $n_4 = 41$, 42 and 43.

4. Discussion

The results for the DCS are consistent with previous calculations. More realistic choices of $2w_1$ and $2w_4$ (100 and 67 μs, respectively), corresponding to the maximum open times of the DCS counter-rotating chopper pairs spinning at ≈ 333 Hz, yield no contaminant regions with $\Delta\lambda < 80$ Å. Given additional considerations, such as the inherent behavior of a counter-rotating chopper pair as a broad band velocity selector [8,11,12], the positioning of the DCS choppers is perfectly acceptable. Our experience to date confirms this conclusion.

Our results for the CNCS are not fully consistent with those of Ref. [9]. For all three choices of the distance d_{13}, we find contamination at relatively short wavelength differences $\Delta\lambda$, whereas Narehood et al. [9] found that the systems with $d_{13} = 7$ m and $d_{13} = 24$ m were both clean. We believe that the present method of calculation is superior to the simulation approaches employed in Ref. [9], and we believe that the present results are correct. The acceptance diagram method tracks areas in (t, τ) (or (t, λ)) phase space, whereas simulations track points. Thus it can be difficult, using a simulation technique, to determine whether a particular type of event has very low probability or identically zero probability. The analytical approach does not suffer this disadvantage. Narehood et al. (private communication, 2003) have recently written an improved simulation program with which they have found that the systems discussed in Ref. [9] are not completely free of contamination. They have since developed a modified CNCS chopper system design that is believed to be clean.

Schober et al. [8] express the transmission properties of a chopper system as the product of Boolean transmission functions for all possible pairs of choppers. In general, these functions depend on the wavelength difference $\Delta\lambda = |\lambda - \lambda_0|$ and on the relative locations of the choppers. Schober et al. plot these functions in $(\Delta\lambda, x)$ space for a chopper system similar to that of the upgraded IN5 spectrometer. A simple example of this type of plot is shown in Fig. 6. It is clear from this type of plot, and indeed from simple geometric considerations, that distance ratios such as d_{12}/d_{13} should not be ratios of small integers. To the author's knowledge, this conclusion has been generally accepted as the "conventional wisdom" since Lowde's original paper on the subject [1]. It is possibly interesting to remark that Fig. 6 is basically a (τ, x) plot, whereas Figs. 1 and 4 are (t, x) plots and Figs. 2, 3 and 5 are (t, τ) plots.

Schober et al.'s approach [8] can in principle be used to determine suitable locations for a single contaminant removal chopper, though the $(\Delta\lambda, x)$ diagram becomes more and more complex with

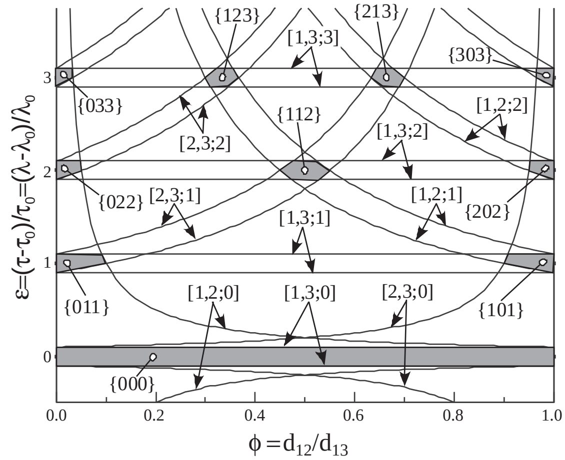

Fig. 6. A plot of the normalized wavelength difference $\varepsilon = (\tau - \tau_0)/\tau_0 = (\lambda - \lambda_0)/\lambda_0$ as a function of the fractional distance $\phi = d_{12}/d_{13}$ for a system of three choppers with identical periods T and open times $2w$, phased to transmit neutrons with wavelength λ_0 (inverse velocity τ_0). Horizontal, positively sloped, and negatively sloped line pairs (with $\varepsilon > 0$) define ε bounds for neutrons transmitted by choppers 1 and 3, 2 and 3, and 1 and 3, respectively. These bounds are defined by the equations $\varepsilon = (n_{\ell k}T \pm 2w)/d_{k\ell}\tau_0$, where $n_{\ell k} = n_\ell - n_k$ and the integer n_k identifies the time that a burst of neutrons passes through chopper k (cf. Fig. 1). Line pairs are labeled with the triplet $[k, \ell; n_{\ell k}]$. For any given value of ϕ, a neutron is transmitted by the chopper system if ε is such that the point (ε, ϕ) lies within one of the hatched areas. These areas are labeled with the triplet $\{n_{12}, n_{23}, n_{13}\}$.

increasing $\Delta\lambda$. The approach may also be used when there is more than one contaminant removal chopper, but the results of such an analysis are considerably harder to visualize since the Boolean transmission functions now depend on more than one distance ratio. For example, a system with two contaminant removal choppers is described using Boolean functions that should ideally be plotted in a three-dimensional space, complicating both the presentation and the interpretation of the results.

The transmission properties of a multiple chopper system are largely independent of the speeds of the choppers, provided the ratios of the speeds are not changed. Furthermore, they depend on the wavelength difference $\Delta\lambda$ and are, to a good approximation, independent of the desired wavelength λ_0 [2,8,10]. Schober et al. [8] provide a helpful discussion of the nature and extent of effects that lead to departures from these simple approximations.

With the advent of a new generation of pulsed neutron sources, there are plans to design and build a number of new neutron scattering instruments, including direct geometry multiple chopper spectrometers. It is imperative that these instruments be designed to produce contaminant-free neutron beams at the sample. To determine the transmission properties of a chopper system, both analytical calculations and ray-tracing simulations should be performed. Generally speaking, the analytical work should precede the simulations since the analytical calculations are fast and essentially exact within the constraints of a simplified description of the instrument. They should be supplemented by Monte Carlo calculations as a check, and as a means to include complicating factors that are necessarily omitted from the analytical calculations.

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References

[1] R.A. Lowde, J. Nucl. Energy, (Part A) 11 (1960) 69.
[2] R. Scherm, T. Springer, Unpublished Report of ILL Grenoble, 1967.
[3] R.E. Lechner, in: Neutron Scattering in the 'Nineties, IAEA, Vienna, 1985, pp. 401–407;
R.E. Lechner, F. Douchin, Y. Blanc, R. Scherm, Unpublished Internal Reports of ILL Grenoble and KFA Jülich, 1973;
see also M. Bée, Quasielastic Neutron Scattering, Adam Hilger, Bristol, 1988 pp. 81–85.
[4] S. Hautecler, E. Legrand, L. Vansteelandt, P. d'Hooghe, G. Rooms, A. Seeger, W. Schalt, G. Gobert, in: Neutron Scattering in the 'Nineties, IAEA, Vienna, 1985, pp. 211–215.
[5] R.E. Lechner, Physica B 180 & 181 (1992) 973.
[6] R.E. Lechner, R. Melzer, J. Fitter, Physica B 226 (1996) 86;
B. Rufflé, J. Ollivier, S. Longeville, R.E. Lechner, Nucl. Instr. and Meth. A 449 (2000) 322.
[7] J.R.D. Copley, J.C. Cook, Chem. Phys. (2003), in press.
[8] H. Schober, Ch. Losert, F. Mezei, J.C. Cook, J. Neut. Res. 8 (2000) 175.
[9] D.G. Narehood, J.V. Pearce, P.E. Sokol, Nucl. Instr. and Meth. A 489 (2002) 337.
[10] J.R.D. Copley, J. Neut. Res. 1 (1993) 21.
[11] J.R.D. Copley, Nucl. Instr. and Meth. A 303 (1990) 332.
[12] J.R.D. Copley, Physica B 180 & 181 (1992) 914.